OMNO2 README File

Version 3.0: September 21, 2006

Overview

Nitrogen dioxide is an important chemical species in both the stratosphere, where it plays a key role in ozone chemistry, and in the troposphere, where it is a precursor to ozone production. In the troposphere, it is produced in various combustion processes and in lightning. It is a significant indicator of poor air quality, and its measurement is a key objective of the OMI project.

This document provides a brief description of the OMI Nitrogen Dioxide (NO_2) data product, OMNO2. The present revision of this document refers to the Public Release of this data product, September 2006. OMNO2 contains slant column NO_2 (total amount along the optical path from the sun into the atmosphere, and then toward the satellite), the total vertical column NO_2 [cm^{-2}], and the estimated tropospheric contribution to the total column NO_2 [cm^{-2}]. Other ancillary data are also provided in the OMNO2 file, including data quality flags, measures of precision, quality assurance (QA) information.

An estimate of the NO_2 column hidden by any clouds in the OMI field of view has been included in the OMNO2 data product for the Public Release. At the user's discretion, this "ghost column" can be added to any of the observed column amounts (defined below in the section "Description of Retrieved NO_2 Columns") to estimate complete column amounts above ground. The ghost column is not a tabulated a priori amount, but is computed from the magnitude of the measured NO_2 column and the assumed a priori NO_2 profile *shape*. Uncertainties in the ghost column are typically large – on the order of 100%.

Application

This document applies to the current public release of the OMNO2 product, version 1.0, September 2006. This product is archived as ECS Collection 2. The software versions used to produce the data are presented in the table below.

OMCLDO2	V1.0.1.1
OMNO2A	V0.9.41.3
OMNO2B	V1.0.0
OMNO2	V0.9.33

Algorithm Description

The basic algorithm for the retrieval of total column and tropospheric NO_2 from OMI data is described by *Boersma et al*. [2001] in *Volume IV* of the *OMI Algorithm Theoretical Basis Document* (ATBD), available at

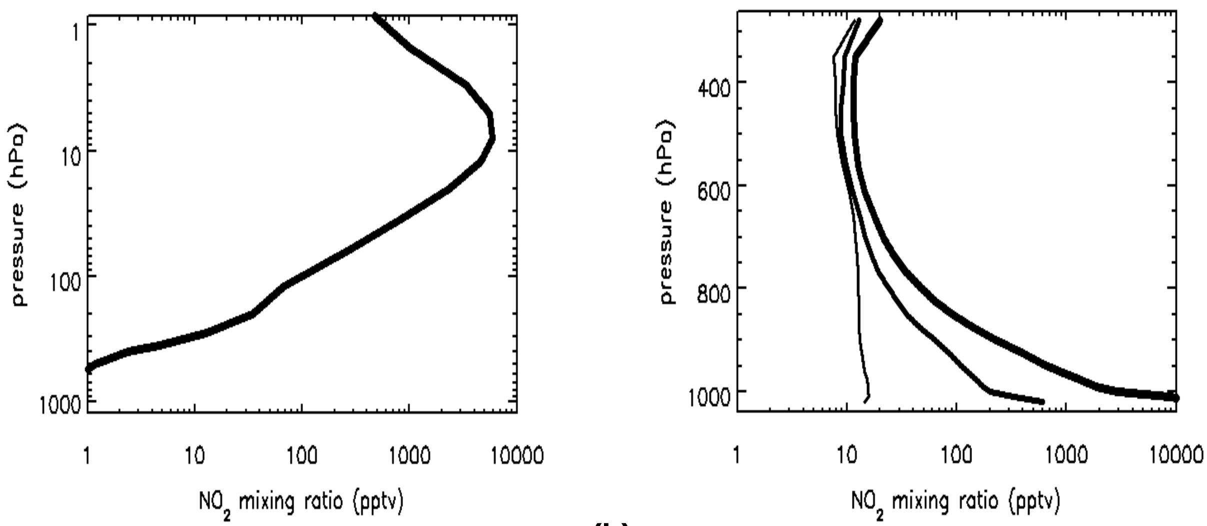
http://eospso.gsfc.nasa.gov/eos_homepage/for_scientists/atbd/docs/OMI/ATBD-OMI-04.pdf

Further information about the algorithm and its development may also be found in *Bucsela et al.,* [2006]. However, some of the data fields in the OMNO2 product differ from those described in these references (see "Description of Retrieved NO_2 Columns" below).

The user is strongly advised to read the section "**Known Issues**" below. The algorithm is divided into three processes, each performed by a separate program, or Product-Generating Executive (*PGE)*. The end result is the creation of the OMNO2 data product from the OMI Level 1B product. Here we briefly describe each PGE.

The first PGE (PGE-A) performs a least-squares fit based on the ratio of the measured earthshine radiance spectrum to a solar irradiance spectrum. A daily OMI measurement of the solar spectrum is normally used to compute the ratio. The closest in time available solar spectrum measurement is used. Information about which solar spectrum was used to process a particular OMI granule is available in the metadata. The functions fitted to the spectral ratio are laboratory-measured trace gas spectra, a reference Ring spectrum [*Chance and Spurr*, 1997] and the coefficients of a polynomial function to model the spectrally slowly varying components of scattering by clouds and aerosols and reflection by the Earth's surface. The fitting algorithm uses the Differential Optical Absorption Spectroscopy (DOAS) method, and is applied in the spectral range 405nm to 465nm. In the current version, the only trace gas absorption spectra considered are those of NO_2 [*Vandaele et al.,* 1998] and O_3 [*Burrows, et al.*, 1999]. The trace gas absorption spectra actually used were produced by convolving high-resolution, laboratory-measured absorption spectra with the measured OMI slit function. The result of the spectral fit is a slant column density (SCD) for each OMI pixel.

The second PGE (PGE-B) computes the air-mass factors (AMFs), defined as the ratio of the SCD to the vertical column density (VCD) of NO_2. AMFs depend upon a number of parameters including viewing geometry, surface albedo and the shape (not magnitude) of the NO_2 vertical profile. AMFs are calculated using both ***unpolluted*** (stratospheric and a small amount of upper tropospheric) and ***polluted*** (lower tropospheric) NO_2 profiles. For each location, the algorithm uses a single mean unpolluted profile derived from the GSFC-CTM and a geographically gridded set of annual mean polluted profiles obtained from the GEOS-CHEM model (see Fig. 1). The method of calculation is similar to that described by *Palmer, et al.* [2001], and uses pre-calculated altitude-dependent AMFs, which are stored in look up tables. For each profile, AMFs are derived for clear and cloudy conditions. Clouds are represented as opaque Lambertian reflectors with an albedo of 0.8. A radiance-weighted sum of the two is used for partly cloudy conditions. The cloud information (cloud fraction and cloud pressure) is obtained from the OMCLDO2 cloud product. The AMFs will be applied in the third PGE to convert the SCDs into VCDs.



(a) **(b)**

Figure 1*: NO_2 concentration profiles used in the calculation of the air mass factors (AMFs). Shown are the unpolluted profile (a) and three examples of polluted profiles (b) for low, moderate and high levels of pollution.*

The third PGE (PGE-C) derives an initial estimate of the NO_2 VCD, V_{init}, by dividing the SCD by an unpolluted AMF, and assembles all the data collected within ±12 hours of the target orbital data granule. Areas shown by GEOS-CHEM to contain climatologically high tropospheric NO_2 amounts are then masked, and the remaining regions are smoothed in latitude bands. The smoothing algorithm employs a "boxcar" smoothing over a 9° latitude band, followed by a zonal planetary wave smoothing up to wave-2. At a given geographic location, the OMI pixels selected for the smoothing are those with the smallest AMFs and slant-column uncertainties. The result is the column amount V_u, which represents the smoothly varying background level of NO_2,including the tropospheric background contribution, and is used in the algorithm as an upper limit on the unpolluted NO_2 column. Pixels for which V_{init} exceeds V_u are assumed to be polluted. The polluted VCD, V_p, is calculated as the difference $V_{init} - V_u$ times the ratio of the unpolluted AMF to the polluted AMF for the pixel. The total column for that pixel is then the sum of V_p and V_u. For all other pixels, the total column is taken to be V_{init}.

Description of Retrieved NO_2 Columns

The Level-2 data file in the Public Release contains four main types of NO_2 vertical column amounts.

(1) *ColumnAmountNO2* (V^{obs})= the total observed vertical column density above ground.
(2) *ColumnAmountNO2Trop* (V_{trop}^{obs})= tropospheric observed vertical column density (integrated from ground to 150 mb).

(3) *ColumnAmountNO2Polluted* (V_p^{obs})= polluted observed vertical column density (integrated from ground to 250 mb).

(4) *ColumnAmountNO2BelowCloud* (V_{ghost}) *= vertical column density hidden by clouds.*

In these definitions, the term *observed* refers to the amount of NO_2 that can be seen from above the atmosphere. The observed amount depends on the vertical distribution of NO_2, the pressure level of the cloud top and the effective cloud fraction. For example, if the effective cloud fraction (based on an assumed 80% cloud albedo) is 50%, then the observed column is half the column density above ground plus half the column density above the cloud top. The Level-2 data also contains an estimate of the column amount below any clouds in the field of view. This amount is sometimes called the "ghost column", and is named *ColumnAmountNO2BelowCloud* in the OMNO2 data product. Adding the ghost column, V_{ghost}, to any observed column amount gives the corresponding complete column between the ground and the satellite, e.g.

$$V_{trop} = V_{trop}^{obs} + V_{ghost}$$

The quantity *ColumnAmountNO2Polluted* is given only in cases where NO_2 exceeds background levels ($V_{init} - V_{smooth} > 0$). In all other cases, fill values are stored. The fill value is the OMI standard fill value, equal to -2^{100}. *ColumnAmountNO2Polluted* is the magnitude of the column above the background, computed assuming that the origin of the excess NO_2 is pollution. Models show pollution affects altitudes mainly below about 250 mb. *ColumnAmountNO2Trop* is defined as the NO_2 vertical column between ground and the estimated mean tropopause pressure of 150 mb. It is obtained by adding 5% (*TropFractionUnpolluted*) of the difference between the total and polluted columns to the polluted column.

Although not given explicitly, the *unpolluted* and *stratospheric* columns can be found by subtracting, respectively, the polluted and tropospheric columns from the total column. Note that for cases of measurable pollution ($V_{init} - V_{smooth} > 0$), the unpolluted column amount is also equal to V_{smooth}. For all other cases, the unpolluted column is defined to be the total column (which is also the initial column in such cases). The VCDQualityFlags data item contains a one-bit flag that indicates whether each pixel was treated as polluted or unpolluted.

Note that the NO_2 fields described here are somewhat different from those discussed in Bucsela et al. [2006], In that document, the unpolluted column amount is referred to as "stratospheric" NO_2, and the polluted column amount is called "tropospheric" NO_2. In the OMNO2 data product, tropospheric NO_2 means the polluted amount plus the 5% of the unpolluted column. Another difference is that *Bucsela et al.* present a direct method for retrieving the complete above-ground column amounts. In OMNO2, only the *observed* columns are retrieved. The complete columns are obtained by adding the ghost column to the total, tropospheric and polluted columns, as described above.

Data Quality Assessment

The quality of the data in this Public Release is currently being established by independent measurements in ongoing validation campaigns from ground-, aircraft-, and satellite-based instruments. Data quality issues are described in the Data Quality document found at http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_quality.pdf
An overview of some of the validation efforts may be found in the presentation http://earth.esa.int/workshops/atmos2006/participants/330/pres_330_kroon.pdf.
Stratospheric amounts are in reasonable agreement with climatological measurements from the Halogen Occultation Experiment (HALOE) instrument aboard the Upper Atmosphere Research Satellite (UARS) and with model calculations from the NASA/GSFC chemical transport model (CTM). Tropospheric amounts are generally consistent with the GEOS-CHEM model and indicate prominent sources near urban areas.

The data product includes estimates of uncertainties associated with the various geophysical quantities. The uncertainty estimates have been improved since the provisional release of the OMI data. However, these estimates may not account for all actual sources of random or systematic errors. We anticipate further improvements through the validation process and in understanding the probability distributions of the underlying data and the algorithmic sensitivity to the data.

Known Issues

As a result of unforeseen characteristics of the OMI CCD detector, most retrieved data products show a varying cross-track anomaly: The average value along any orbital track at one cross-track position may differ significantly from that along nearby cross-track positions, resulting in the appearance of "stripes" when the data are displayed on a map. The origin of this artifact is almost certainly in the performance of the CCD detectors themselves; a suitable correction to the measured solar irradiances and earthshine radiances has been developed and will be implemented in the next release of the Level 1B data (collection 3). In the current release the striping in the retrieved data can only be removed in a *post-hoc* fashion.

The OMNO2 algorithm has been fitted with a module, used in the third PGE, that performs a "de-striping" of NO_2 column amounts by adjusting the mean SCD for a given cross-track position to the mean value at all positions. The current version of the de-striping algorithm computes the mean SCD and the mean initial AMF for each cross-track position from 24-hours of data using measurements obtained at latitudes between ±55°. These are used to generate a set of 60 correction constants, one for each cross-track position, which are subtracted from the SCD values before computation of the vertical columns. The user should note that the slant columns (*SlantColumnAmountNO2*) actually stored in the Level-2 file are from the original spectral fit and have *not* been de-striped. However the all stored vertical columns, with the exception of *ColumnAmountNO2Initial*, have been de-striped.

The de-striping procedure will almost certainly introduce an unknowable systematic bias in the retrieved NO_2 VCDs, which could vary from orbit to orbit. As mentioned above, we anticipate that as the understanding of the instrumental artifact evolves, the OMI Level 1B product will ultimately contain consistent, calibrated radiances and irradiances, which will lead to retrieved NO_2 VCDs that do not show a cross-track dependence. This will eliminate the need for *post-hoc* corrections.

The air mass factors are computed in PGE-B using a look-up table from radiative transfer calculations. The calculations are performed on a 6-dimensional grid of pressures, solar zenith angles, viewing zenith angles, relative azimuth angles, albedos and surface pressures, and the algorithm interpolates between grid points. A finer grid is planned for implementation in the next version of the algorithm. Use of the current coarse grid can cause errors in the polluted AMF, and hence the retrieved polluted and tropospheric column amounts, as large as10% relative to the fine grid.

An OMI instrument anomaly required that a fixed OMI solar irradiance measurement be used in PGE-A from February 2006 through July 2006. A daily solar spectrum is normally used in the retrieval, but a reference solar spectrum is being developed for future implementation in the algorithm.

The user is referred to the **Release Notes** for additional information and cautions pertaining to the use and interpretation of the data:
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_release_notes.pdf.

Product Description

A single OMNO2 product file contains all OMI measurements on the sunlit portion of the Earth, for one Aura orbit. During one orbit OMI performs approximately 1650 measurements, which take 2 seconds each. In the global observation mode, 60 across track ground pixels are measured simultaneously during a measurement. These 60 measurements cover the ~2600 km-wide OMI ground swath. Fig. 2 shows that due to optical aberrations and the asymmetric alignment between the instrument's optical axis and the spacecraft axes, the ground pixels are not symmetrically aligned with respect to the orbital plane.

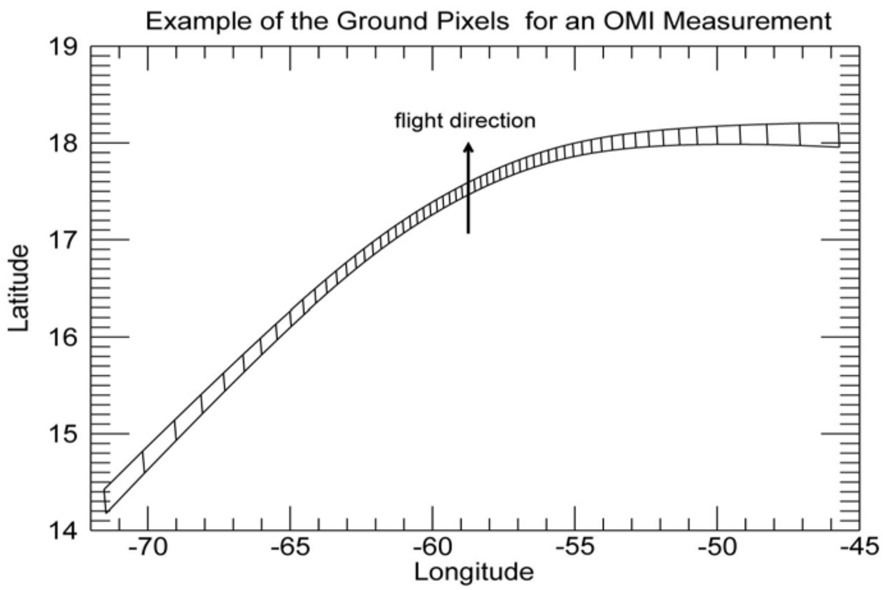


Figure 2*: The position of 60 ground pixels for an OMI measurement in the tropics. Note that the x and y axes cover different distances on the Earth's surface. The arrow shows the satellite trajectory*

The latitude and longitude provided with each ground pixel represent the location of the center of each pixel on the ground. Fig. 3 gives the size of the ground pixels, as a function of pixel number in the across track direction. Although the pixels also increase in the flight direction when going off nadir, this effect is much smaller and may be neglected for most applications.

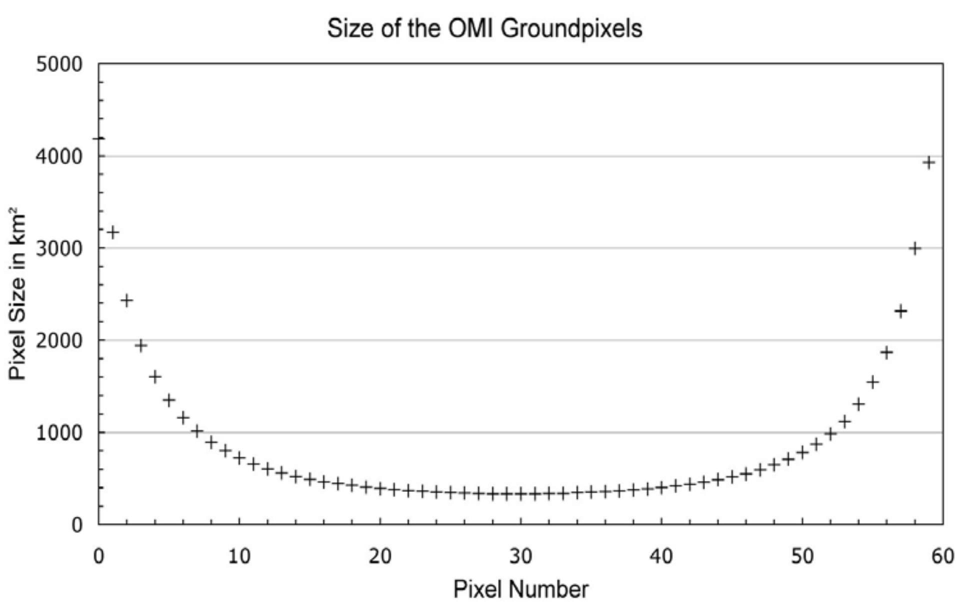


Figure 3*: The size of the OMI ground pixels, as a function of the across track pixel number*

The OMNO2 product is written as an HDF-EOS5 swath file. For a list of tools that read HDF-EOS5 data files, please visit this link:

http://disc.gsfc.nasa.gov/Aura/tools.shtml,

A single OMNO2 file contains information retrieved from each OMI pixel over the sun-lit portion of one Aura orbit. The data are ordered in time. The information provided in these files includes latitude, longitude, a set of viewing angles (solar zenith and solar azimuth; viewing zenith and viewing azimuth), column amounts of NO_2, intermediate quantities used in the calculation, such as AMFs and coefficients of the smooth NO_2 field, and a large number of ancillary parameters that provide information to assess data quality. Among the latter are several data quality flag fields (ground pixel quality, measurement quality, fit quality, AMF quality, and unpolluted field quality). These should be examined to assess the quality of individual measurements, particularly for inter-comparison studies. A summary flag is also provided to indicate the overall quality of the data for a given pixel. A value of 0 for this flag indicates the best quality data, a value of 2 is for poor quality data and a value of 3 is given to data that should not be used. The value of 1 is not currently defined. For a complete list of fields and ancillary data contained in the OMNO2 file, please read the OMNO2 data product specification http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_product_specification.pdf.

For users not interested in the detailed information provided in OMNO2 dataset, we are developing several gridded products. Full OMNO2 data, as well as subsets of these data over many ground stations and along Aura validation aircraft flights paths are available to those investigators who are associated with the various Aura science teams through the Aura Validation Data Center (AVDC) website, http://avdc.gsfc.nasa.gov/. Bojan Bojkov Bojan.Bojkov@avdc.gsfc.nasa.gov is the point of contact at the AVDC.

Reporting Problems and Requesting Information

The following is a summary of links to current documentation for OMNO2:

http://toms.gsfc.nasa.gov/omi/no2/OMNO2_readme.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_release_notes.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_quality.pdf
http://toms.gsfc.nasa.gov/omi/no2/OMNO2_data_product_specification.pdf

To report problems, or pose questions and comments related to the OMNO2 algorithm, data quality, and file structure, please send electronic mail to omno2@ltpmail.gsfc.nasa.gov. Additional questions may be directed to the principal points of contact for OMNO2: James F. Gleason gleason@redwind.gsfc.nasa.gov, and J. Pepijn Veefkind veefkind@knmi.nl.

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